



wwPDB/EMDatabank EM Map/Model Validation Summary Report ⓘ

Jul 24, 2017 – 04:47 AM EDT

PDB ID : 5NP6
EMDB ID: : EMD-3618
Title : 70S structure prior to bypassing
Authors : Agirrezabala, X.; Samatova, E.; Klimova, M.; Zamora, M.; Gil-Carton, D.;
Rodnina, M.; Valle, M.
Deposited on : unknown
Resolution : 3.60 Å(reported)

This is a wwPDB/EMDatabank EM Map/Model Validation Summary Report
for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20029824

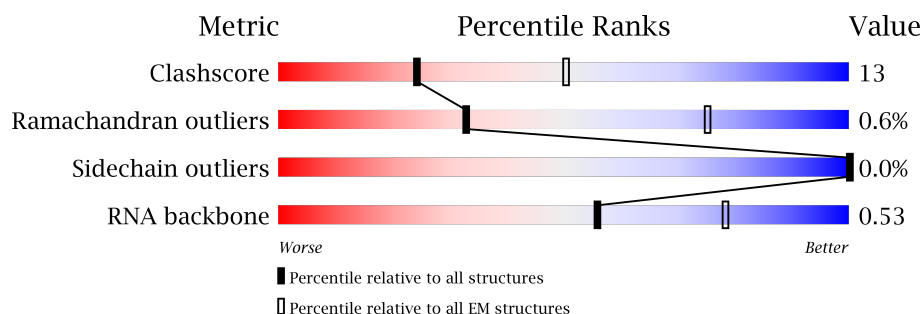
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



















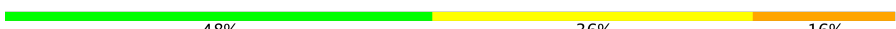

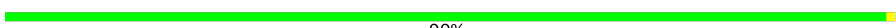
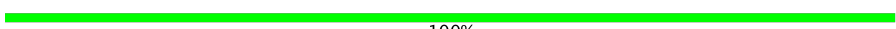
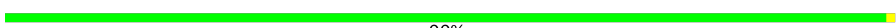

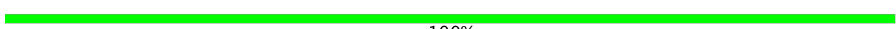
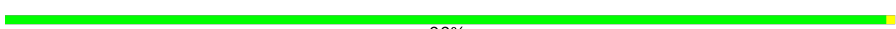

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026
RNA backbone	3398	335

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	29	10% 34% 48% 7%
2	B	76	42% 39% 18%
3	C	46	41% 57% .
4	D	1539	50% 37% 13%
5	E	218	67% 33%
6	F	206	82% 18%
7	G	205	66% 34%
8	H	157	69% 29% .

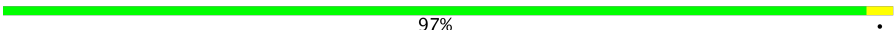
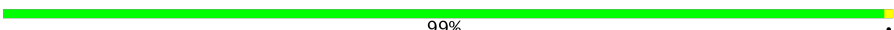
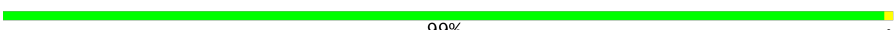
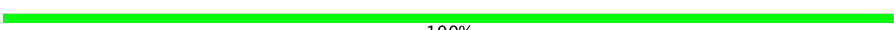
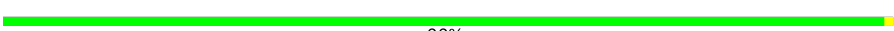







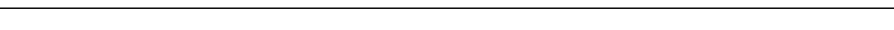
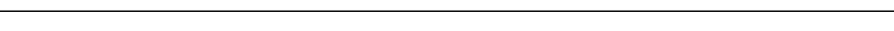
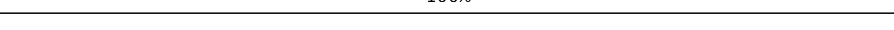
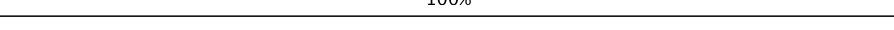
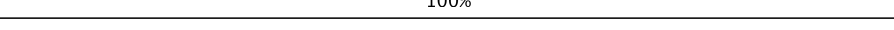
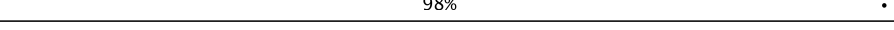
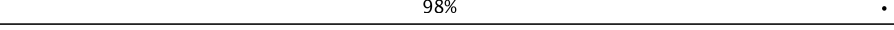
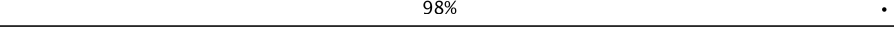




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Mol	Chain	Length	Quality of chain
9	I	100	 64% 35% .
10	J	151	 69% 31%
11	K	129	 74% 26%
12	L	127	 60% 39% .
13	M	98	 57% 42% .
14	N	116	 66% 33% .
15	O	123	 77% 23%
16	P	114	 74% 26%
17	Q	101	 69% 31%
18	R	88	 84% 16%
19	S	82	 76% 24%
20	T	80	 76% 24%
21	U	65	 71% 28% .
22	V	79	 77% 23%
23	W	85	 68% 31% .
24	X	65	 66% 32% .
25	Y	2903	 48% 36% 16%
26	Z	120	 52% 33% 14% .
27	a	271	 99% .
28	b	209	 100%
29	c	201	 99% .
30	d	177	 100%
31	e	176	 100%
32	f	149	 99% .
33	g	141	 98% .

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Mol	Chain	Length	Quality of chain
34	h	142	 97% .
35	i	122	 99% .
36	j	143	 99% .
37	k	136	 100%
38	l	120	 99% .
39	m	116	 99% .
40	n	114	 99% .
41	o	117	 100%
42	p	103	 99% .
43	q	110	 100%
44	r	93	 100%
45	s	102	 100%
46	t	94	 100%
47	u	75	 100%
48	v	77	 100%
49	w	63	 100%
50	x	58	 98% .
51	y	56	 98% .
52	z	50	 98% .
53	0	46	 63% 37%
54	1	64	 80% 20%
55	2	38	 82% 18%
56	3	131	 41% 56% .
57	4	66	 64% 36%

2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 146883 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	29	Total	C	N	O	P	0	0
			621	277	111	204	29		

- Molecule 2 is a RNA chain called P-site tRNA-Gly.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	76	Total	C	N	O	P	0	0
			1623	722	291	534	76		

- Molecule 3 is a protein called DNA topoisomerase small subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	46	Total	C	N	O	S	0	0
			362	222	65	71	4		

- Molecule 4 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	1539	Total	C	N	O	P	0	0
			33028	14738	6052	10699	1539		

- Molecule 5 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	218	Total	C	N	O	S	0	0
			1704	1081	305	311	7		

- Molecule 6 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	206	Total	C	N	O	S	0	0
			1624	1028	305	288	3		

- Molecule 7 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	205	Total	C	N	O	S	0	0
			1643	1026	315	298	4		

- Molecule 8 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	157	Total	C	N	O	S	0	0
			1141	709	218	208	6		

- Molecule 9 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	100	Total	C	N	O	S	0	0
			817	515	148	148	6		

- Molecule 10 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	151	Total	C	N	O	S	0	0
			1181	735	227	215	4		

- Molecule 11 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	129	Total	C	N	O	S	0	0
			979	616	173	184	6		

- Molecule 12 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	127	Total	C	N	O	S	0	0
			1022	634	206	179	3		

- Molecule 13 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	98	Total	C	N	O	S	0	0
			786	493	150	142	1		

- Molecule 14 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	116	Total	C	N	O	S	0	0
			869	535	173	158	3		

- Molecule 15 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	123	Total	C	N	O	S	0	0
			955	590	196	165	4		

- Molecule 16 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	114	Total	C	N	O	S	0	0
			883	546	178	156	3		

- Molecule 17 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	101	Total	C	N	O	S	0	0
			799	498	165	133	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	35	ALA	-	insertion	UNP P0AG59

- Molecule 18 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	88	Total	C	N	O	S	0	0
			714	439	144	130	1		

- Molecule 19 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	82	Total	C	N	O	S	0	0
			649	406	128	114	1		

- Molecule 20 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	80	Total	C	N	O	S	0	0
			648	411	121	113	3		

- Molecule 21 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	U	65	Total	C	N	O	0	0
			504	317	96	91		

- Molecule 22 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	79	Total	C	N	O	S	0	0
			637	408	120	107	2		

- Molecule 23 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W	85	Total	C	N	O	S	0	0
			665	411	137	114	3		

- Molecule 24 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	X	65	Total	C	N	O	S	0	0
			495	307	100	87	1		

- Molecule 25 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Y	2903	Total	C	N	O	P	0	0
			62338	27816	11471	20148	2903		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Y	747	5MC	U	conflict	GB 802133627
Y	887	A	U	conflict	GB 802133627
Y	1847	G	A	conflict	GB 802133627

- Molecule 26 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Z	120	Total	C	N	O	P	0	0
			2572	1145	471	836	120		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Z	120	A	U	conflict	GB 1146054517

- Molecule 27 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	a	271	Total	C	N	O	S	0	0
			2082	1288	423	364	7		

- Molecule 28 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	b	209	Total	C	N	O	S	0	0
			1565	979	288	294	4		

- Molecule 29 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	c	201	Total	C	N	O	S	0	0
			1552	974	283	290	5		

- Molecule 30 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	d	177	Total	C	N	O	S	0	0
			1410	899	249	256	6		

- Molecule 31 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	e	176	Total	C	N	O	S	0	0
			1323	832	243	246	2		

- Molecule 32 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	f	149	Total	C	N	O	S	0	0
			1111	699	197	214	1		

- Molecule 33 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	g	141	Total	C	N	O	S	0	0
			1032	651	179	196	6		

- Molecule 34 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	h	142	Total	C	N	O	S	0	0
			1129	714	212	199	4		

- Molecule 35 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	i	122	Total	C	N	O	S	0	0
			938	587	180	165	6		

- Molecule 36 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	j	143	Total	C	N	O	S	0	0
			1045	649	206	189	1		

- Molecule 37 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	k	136	Total	C	N	O	S	0	0
			1074	686	205	177	6		

- Molecule 38 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	l	120	Total	C	N	O	S	0	0
			960	593	196	166	5		

- Molecule 39 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				AltConf	Trace
39	m	116	Total	C	N	O	0	0
			892	552	178	162		

- Molecule 40 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms				AltConf	Trace
40	n	114	Total	C	N	O	S	0
			917	574	179	163	1	0

- Molecule 41 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms				AltConf	Trace
41	o	117	Total	C	N	O		0
			947	604	192	151		0

- Molecule 42 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms				AltConf	Trace
42	p	103	Total	C	N	O	S	0
			816	516	153	145	2	0

- Molecule 43 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms				AltConf	Trace
43	q	110	Total	C	N	O	S	0
			857	532	166	156	3	0

- Molecule 44 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms				AltConf	Trace
44	r	93	Total	C	N	O	S	0
			738	466	139	131	2	0

- Molecule 45 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
45	s	102	Total	C	N	O		0
			779	492	146	141		0

- Molecule 46 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	t	94	Total	C	N	O	S	0	0
			753	479	137	134	3		

- Molecule 47 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	u	75	Total	C	N	O	S	0	0
			575	356	116	102	1		

- Molecule 48 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	v	77	Total	C	N	O	S	0	0
			625	388	129	106	2		

- Molecule 49 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	w	63	Total	C	N	O	S	0	0
			509	313	99	95	2		

- Molecule 50 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	x	58	Total	C	N	O	S	0	0
			449	281	87	79	2		

- Molecule 51 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	y	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 52 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
52	z	50	Total	C	N	O	0	0
			409	263	75	71		

- Molecule 53 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	0	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 54 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	1	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 55 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	2	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 56 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	3	131	Total	C	N	O	S	0	0
			988	625	175	183	5		

- Molecule 57 is a protein called 50S ribosomal protein L31.

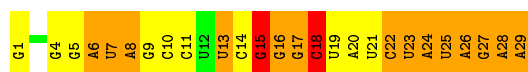
Mol	Chain	Residues	Atoms					AltConf	Trace
57	4	66	Total	C	N	O	S	0	0
			522	323	99	94	6		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: mRNA

Chain A: 



- Molecule 2: P-site tRNA-Gly

Chain B: 



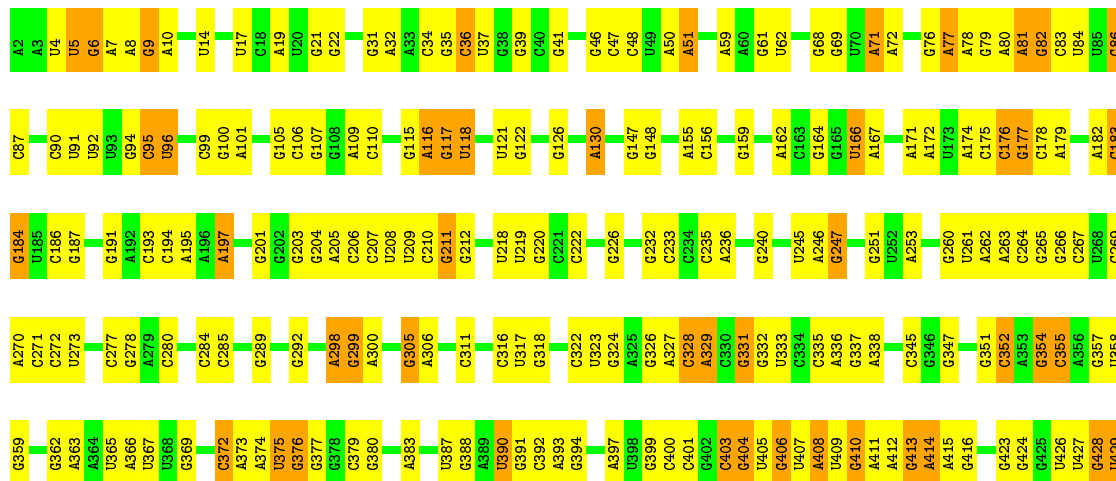
- Molecule 3: DNA topoisomerase small subunit

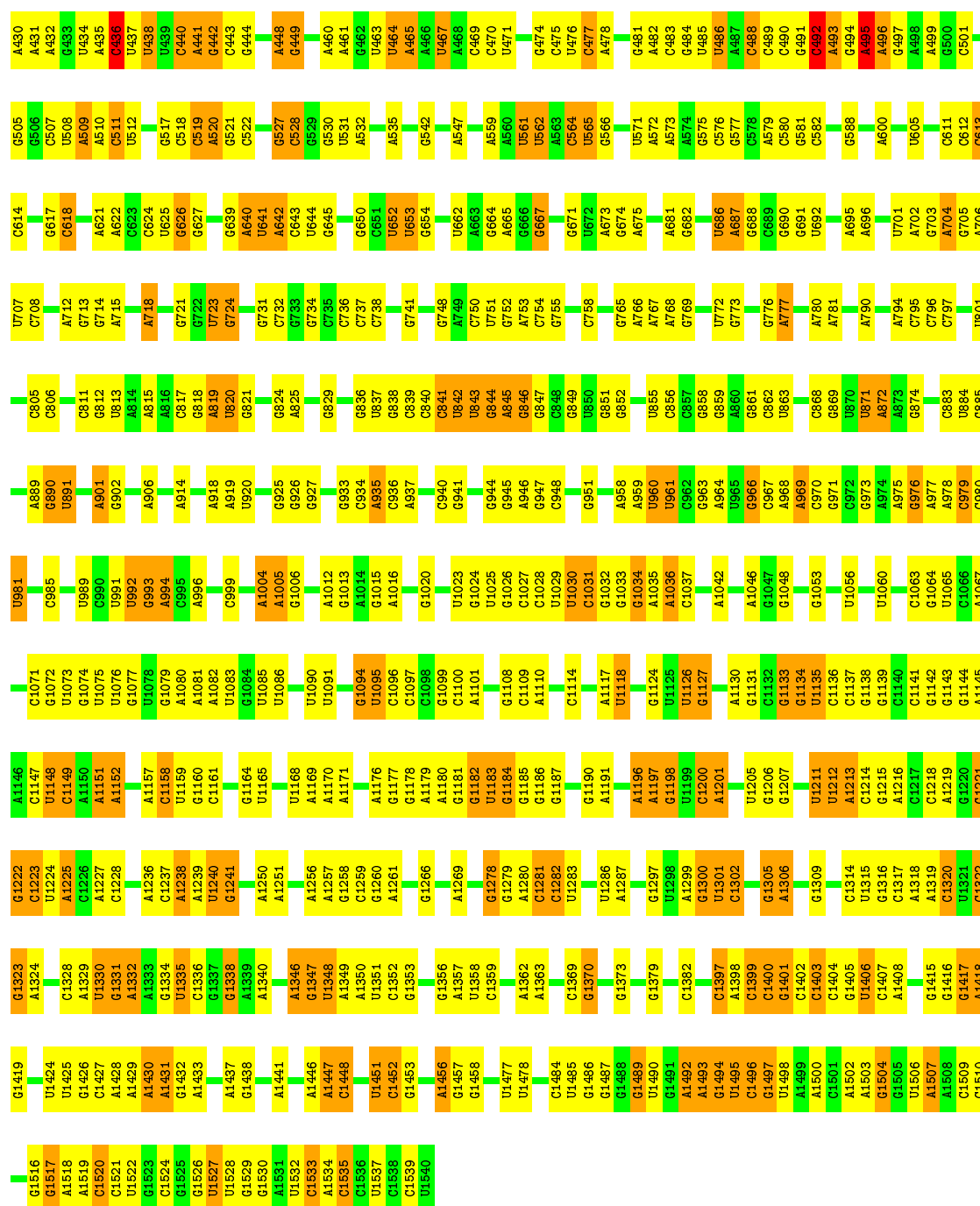
Chain C: 



- Molecule 4: 16S ribosomal RNA

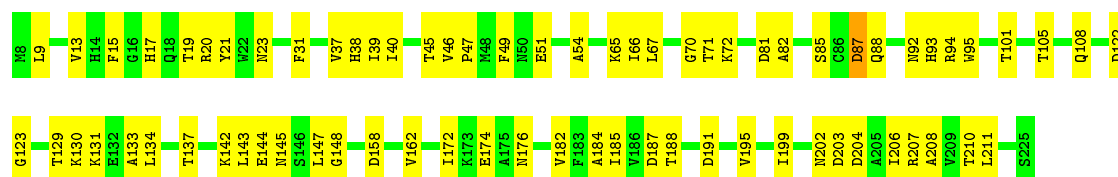
Chain D: 



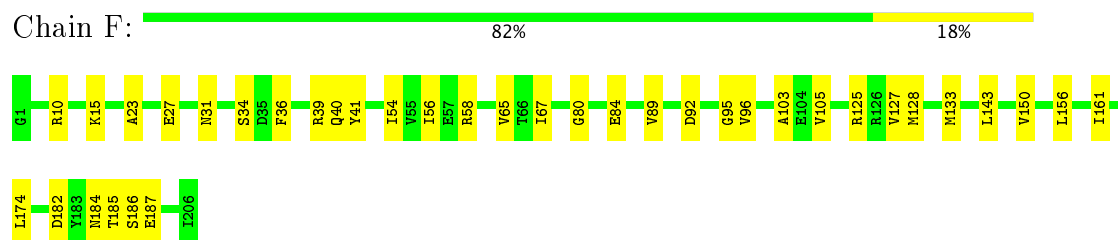


• Molecule 5: 30S ribosomal protein S2

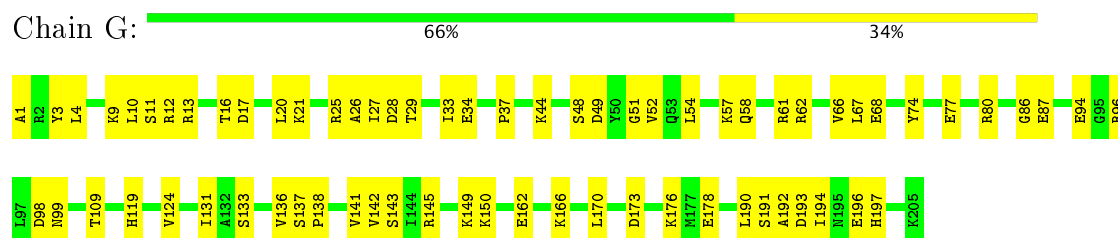
Chain E: 67% 33%



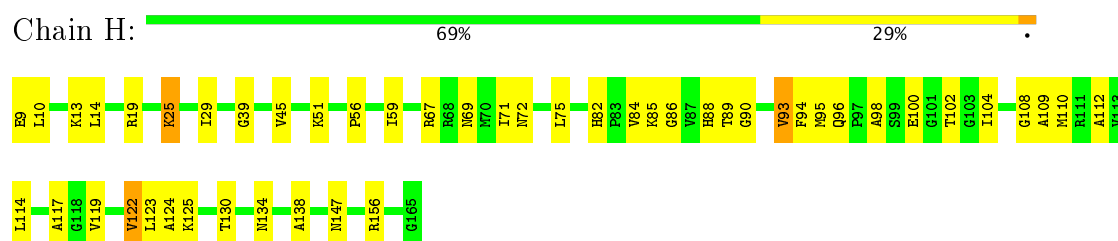
• Molecule 6: 30S ribosomal protein S3



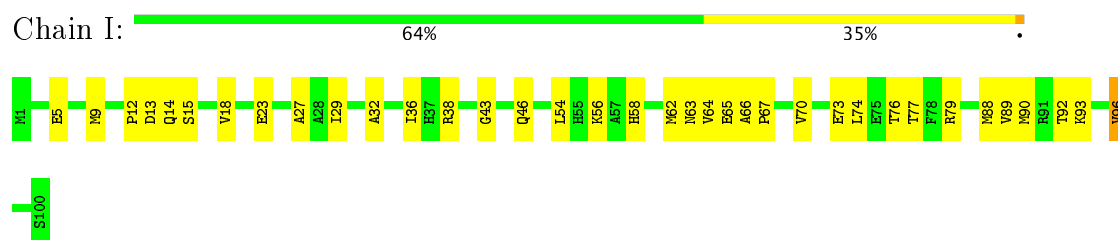
- Molecule 7: 30S ribosomal protein S4



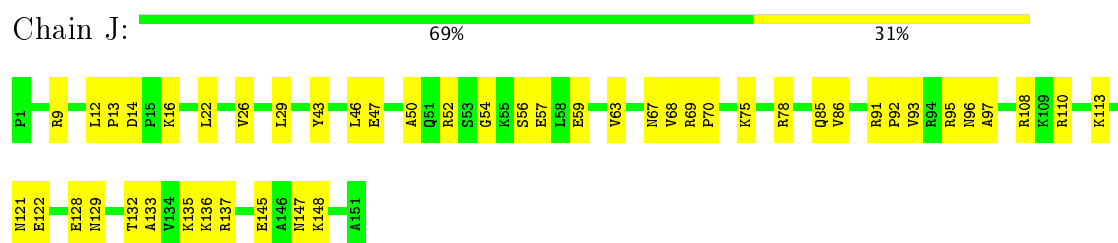
- Molecule 8: 30S ribosomal protein S5



- Molecule 9: 30S ribosomal protein S6



- Molecule 10: 30S ribosomal protein S7



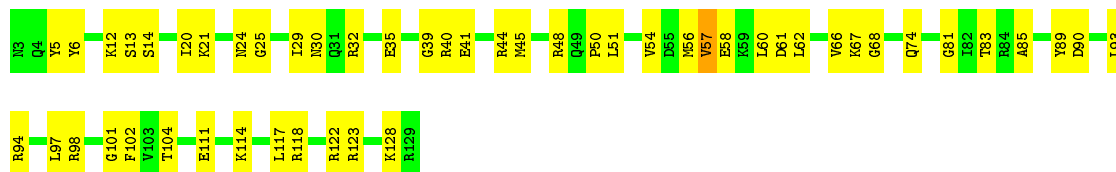
- Molecule 11: 30S ribosomal protein S8





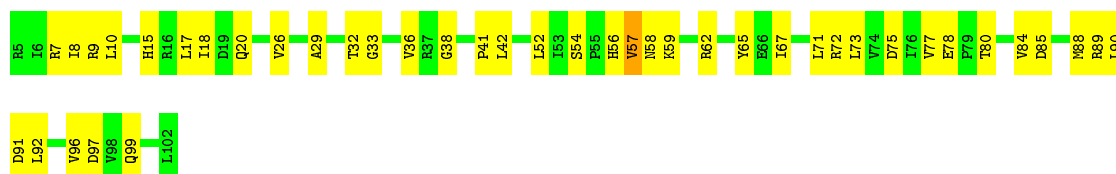
- Molecule 12: 30S ribosomal protein S9

Chain L: 60% 39%



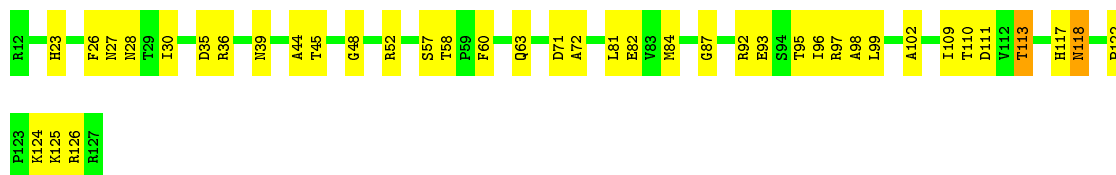
- Molecule 13: 30S ribosomal protein S10

Chain M: 57% 42%



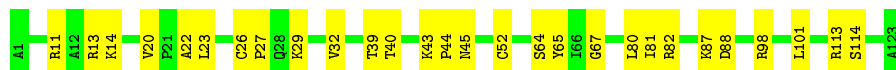
- Molecule 14: 30S ribosomal protein S11

Chain N: 66% 33%



- Molecule 15: 30S ribosomal protein S12

Chain O: 77% 23%



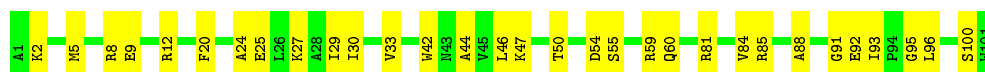
- Molecule 16: 30S ribosomal protein S13

Chain P: 74% 26%



- Molecule 17: 30S ribosomal protein S14

Chain Q: 69% 31%



- Molecule 18: 30S ribosomal protein S15

Chain R: 84% 16%



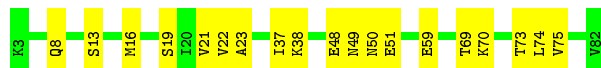
- Molecule 19: 30S ribosomal protein S16

Chain S: 76% 24%



- Molecule 20: 30S ribosomal protein S17

Chain T: 76% 24%



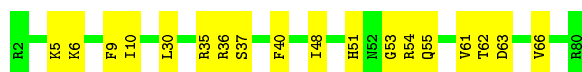
- Molecule 21: 30S ribosomal protein S18

Chain U: 71% 28% .



- Molecule 22: 30S ribosomal protein S19

Chain V: 77% 23%



- Molecule 23: 30S ribosomal protein S20

Chain W: 68% 31% .



- Molecule 24: 30S ribosomal protein S21

Chain X: 66% 32% .

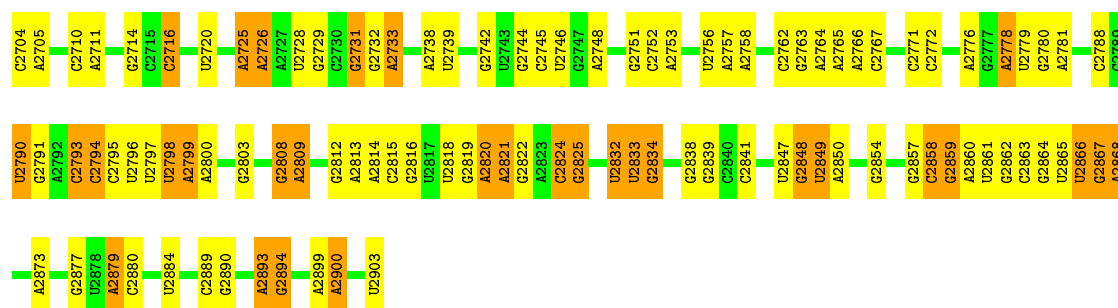


• Molecule 25: 23S ribosomal RNA

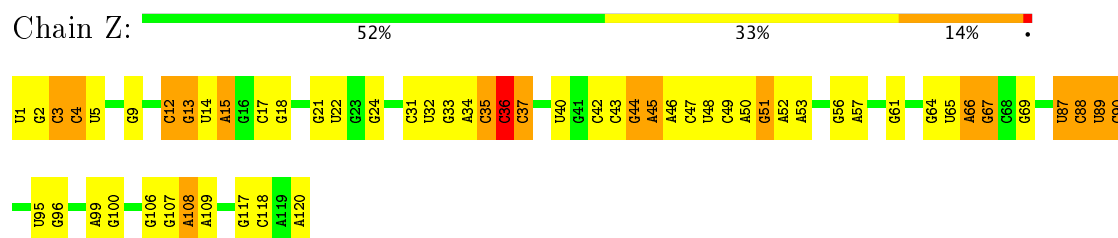
Chain Y: 

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C96	C97	G98	U99	U100	A101	U102	A103	G107	G110	A111	U112	U113	U114	C115	U116	G117	A118	U120	A131	G132	U133	G134	U135	G136	U137	U138	C140	G141	A142	A149	U150	A151	C152	A153	G157	G158	A162	C163	G167	G168	A171	U172	A173	G175	G176	G177	U178	C179	A180	G181	U182	G185	A189	U193	G194	A195	A196						
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C687	G690	U703	G704	A705	U710	G711	A715	A716	C717	G726	A727	G728	U729	A730	C731	U732	G733	A734	U735	C736	G737	G738	U744	G745	U746	C747	U748	A749	U750	A751	A752	U754	U755	U756	U757	U758	U759	U760	A761	U762	G763	A764	C765	G770	U771	U772	U773	U774	U775	U776	U777	U778	U779	U780									
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U868	A878	G882	G883	U887	C888	C889	C890	G891	U894	U895	A896	C897	U898	A899	C903	G904	U907	G908	G909	U910	A911	G914	C915	G923	G924	A925	U926	A927	A928	U929	G930	U931	U932	A933	U941	A945	C946	A947	G953	G954	U955	G956	C957	U958	A959	A960	C961	U963															
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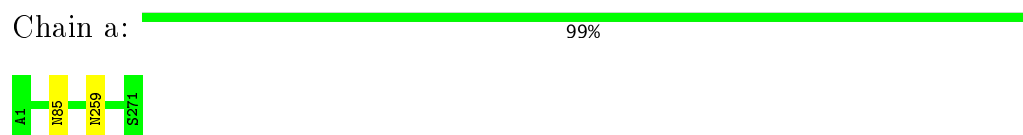
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A2599	A2599	U2521	G2443	A2270	A2169	C2103	C2024	A1931	U1841	A1750	U1657	U1481	A1374	
A2600	A2600	G2522	G2444	G2271	A2170	U2104	G2025	U1932	U1842	A1751	C1664	G1482	G1374	
A2601	A2601	U2523	G2445	U2272	A2171	U2105	U2026	U1933	C1843	A1752	A1664	G1483	G1375	
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A2608	A2608	G2530	G2452	A2279	U2178	U2112	U2033	U1940	C1850	A1759	A1671	G1490	G1382	
A2609	A2609	U2531	G2453	A2280	U2179	U2113	U2034	U1941	C1851	A1760	A1672	G1491	G1383	
A2610	A2610	G2532	G2454	A2281	U2180	U2114	U2035	U1942	C1852	A1761	A1673	G1492	G1384	
A2611	A2611	U2533	G2455	A2282	U2181	U2115	U2036	U1943	C1853	A1762	A1674	G1493	G1385	
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A2613	A2613	U2535	G2457	A2284	U2183	U2117	U2038	U1945	C1855	A1764	A1676	G1495	G1387	
A2614	A2614	G2536	G2458	A2285	U2184	U2118	U2039	U1946	C1856	A1765	A1677	G1496	G1388	
A2615	A2615	U2537	G2459	A2286	U2185	U2119	U2040	U1947	C1857	A1766	A1678	G1497	G1389	
A2616	A2616	G2538	G2460	A2287	U2186	U2120	U2041	U1948	C1858	A1767	A1679	G1498	G1390	
A2617	A2617	U2539	G2461	A2288	U2187	U2121	U2042	U1949	C1859	A1768	A1680	G1499	G1391	
A2618	A2618	G2540	G2462	A2289	U2188	U2122	U2043	U1950	C1860	A1769	A1681	G1500	G1392	
A2619	A2619	U2541	G2463	A2290	U2189	U2123	U2044	U1951	C1861	A1770	A1682	G1501	G1393	
A2620	A2620	G2542	G2464	A2291	U2190	U2124	U2045	U1952	C1862	A1771	A1683	G1502	G1394	
A2621	A2621	U2543	G2465	A2292	U2191	U2125	U2046	U1953	C1863	A1772	A1684	G1503	G1395	
A2622	A2622	G2544	G2466	A2293	U2192	U2126	U2047	U1954	C1864	A1773	A1685	G1504	G1396	
A2623	A2623	U2545	G2467	A2294	U2193	U2127	U2048	U1955	C1865	A1774	A1686	G1505	G1397	
A2624	A2624	G2546	A2468	A2295	U2194	U2128	U2049	U1956	C1866	A1775	A1687	G1506	G1398	
A2625	A2625	U2547	G2469	A2296	U2195	U2129	U2050	U1957	C1867	A1776	A1688	G1507	G1399	
A2626	A2626	G2548	G2470	A2297	U2196	U2130	U2051	U1958	C1868	A1777	A1689	G1508	G1400	
A2627	A2627	U2549	G2471	A2298	U2197	U2131	U2052	U1959	C1869	A1778	A1690	G1509	G1401	
A2628	A2628	G2550	G2472	A2299	U2198	U2132	U2053	U1960	C1870	A1779	A1691	G1510	G1402	
A2629	A2629	U2551	G2473	A2300	U2199	U2133	U2054	U1961	C1871	A1780	A1692	G1511	G1403	
A2630	A2630	G2552	G2474	A2301	U2200	U2134	U2055	U1962	C1872	A1781	A1693	G1512	G1404	
A2631	A2631	U2553	G2475	A2302	U2201	U2135	U2056	U1963	C1873	A1782	A1694	G1513	G1405	
A2632	A2632	G2554	G2476	A2303	U2202	U2136	U2057	U1964	C1874	A1783	A1695	G1514	G1406	
A2633	A2633	U2555	G2477	A2304	U2203	U2137	U2058	U1965	C1875	A1784	A1696	G1515	G1407	
A2634	A2634	G2556	G2478	A2305	U2204	U2138	U2059	U1966	C1876	A1785	A1697	G1516	G1408	
A2635	A2635	U2557	G2479	A2306	U2205	U2139	U2060	U1967	C1877	A1786	A1698	G1517	G1409	
A2636	A2636	G2558	G2480	A2307	U2206	U2140	U2061	U1						



- Molecule 26: 5S ribosomal RNA



- Molecule 27: 50S ribosomal protein L2



- Molecule 28: 50S ribosomal protein L3



There are no outlier residues recorded for this chain.

- Molecule 29: 50S ribosomal protein L4



- Molecule 30: 50S ribosomal protein L5



There are no outlier residues recorded for this chain.

- Molecule 31: 50S ribosomal protein L6



There are no outlier residues recorded for this chain.

- Molecule 32: 50S ribosomal protein L9

Chain f:  99%



- Molecule 33: 50S ribosomal protein L11

Chain g:  98%



- Molecule 34: 50S ribosomal protein L13

Chain h:  97%



- Molecule 35: 50S ribosomal protein L14

Chain i:  99%



- Molecule 36: 50S ribosomal protein L15

Chain j:  99%



- Molecule 37: 50S ribosomal protein L16

Chain k:  100%

There are no outlier residues recorded for this chain.

- Molecule 38: 50S ribosomal protein L17

Chain l:  99%



- Molecule 39: 50S ribosomal protein L18

Chain m:  99%



- Molecule 40: 50S ribosomal protein L19

Chain n:  99%



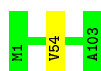
- Molecule 41: 50S ribosomal protein L20

Chain o:  100%

There are no outlier residues recorded for this chain.

- Molecule 42: 50S ribosomal protein L21

Chain p:  99%



- Molecule 43: 50S ribosomal protein L22

Chain q:  100%

There are no outlier residues recorded for this chain.

- Molecule 44: 50S ribosomal protein L23

Chain r:  100%

There are no outlier residues recorded for this chain.

- Molecule 45: 50S ribosomal protein L24

Chain s:  100%

There are no outlier residues recorded for this chain.

- Molecule 46: 50S ribosomal protein L25

Chain t:  100%

There are no outlier residues recorded for this chain.

- Molecule 47: 50S ribosomal protein L27

Chain u:  100%

There are no outlier residues recorded for this chain.

- Molecule 48: 50S ribosomal protein L28

Chain v:  100%

There are no outlier residues recorded for this chain.

- Molecule 49: 50S ribosomal protein L29

Chain w:  100%

There are no outlier residues recorded for this chain.

- Molecule 50: 50S ribosomal protein L30

Chain x:  98%



- Molecule 51: 50S ribosomal protein L32

Chain y:  98%



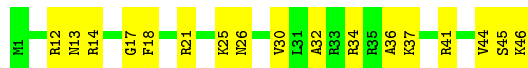
- Molecule 52: 50S ribosomal protein L33

Chain z:  98%




- Molecule 53: 50S ribosomal protein L34

Chain 0:  63% 37%




- Molecule 54: 50S ribosomal protein L35

Chain 1:  80% 20%



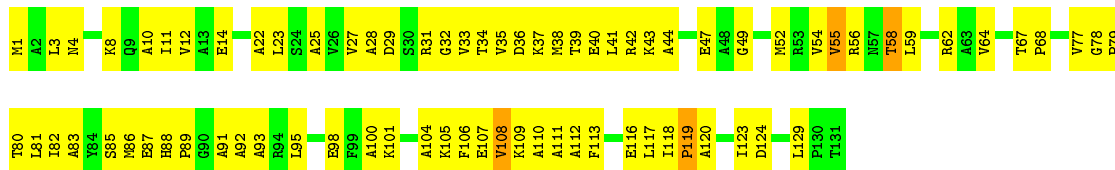
- Molecule 55: 50S ribosomal protein L36

Chain 2:  82% 18%



- Molecule 56: 50S ribosomal protein L10

Chain 3: 41% 56%



- Molecule 57: 50S ribosomal protein L31

Chain 4: 64% 36%



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	36983	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE; CTF correction inside Relion	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	2.66	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	47170	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 5MU, 3TD, OMG, 5MC, MA6, H2U, OMC, 2MA, 6MZ, 2MG, OMU, UR3, 4OC, 7MG, 1MG, PSU

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
1	A	0.97	1/694 (0.1%)	1.52	15/1078 (1.4%)
10	J	0.26	0/1195	0.43	0/1602
11	K	0.37	1/989 (0.1%)	0.50	0/1326
12	L	0.30	0/1034	0.53	0/1375
13	M	0.37	1/796 (0.1%)	0.50	0/1077
14	N	0.35	1/885 (0.1%)	0.51	0/1195
15	O	0.30	0/969	0.50	0/1300
16	P	0.26	0/892	0.46	0/1193
17	Q	0.27	0/811	0.47	0/1081
18	R	0.27	0/722	0.46	0/964
19	S	0.30	0/659	0.49	0/884
2	B	0.38	1/1812 (0.1%)	0.83	0/2822
20	T	0.29	0/657	0.52	0/881
21	U	0.29	0/511	0.49	0/689
22	V	0.27	0/652	0.46	0/877
23	W	0.29	0/671	0.45	0/888
24	X	0.30	0/500	0.53	0/668
25	Y	0.30	2/69244 (0.0%)	0.84	26/108021 (0.0%)
26	Z	0.32	1/2876 (0.0%)	0.81	2/4483 (0.0%)
27	a	0.36	0/2121	0.51	0/2852
28	b	0.28	0/1586	0.49	0/2134
29	c	0.40	1/1571 (0.1%)	0.45	0/2113
3	C	0.29	0/365	0.56	0/485
30	d	0.27	0/1434	0.46	0/1926
31	e	0.26	0/1343	0.47	0/1816
32	f	0.30	0/1122	0.47	0/1515
33	g	0.27	0/1046	0.50	0/1410
34	h	0.27	0/1152	0.46	0/1551
35	i	0.28	0/947	0.49	0/1268
36	j	0.34	0/1054	0.55	0/1403
37	k	0.29	0/1093	0.48	0/1460

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
38	l	0.27	0/973	0.45	0/1301
39	m	0.26	0/902	0.46	0/1209
4	D	0.29	1/36700 (0.0%)	0.82	7/57246 (0.0%)
40	n	0.34	0/929	0.49	0/1242
41	o	0.34	0/960	0.41	0/1278
42	p	0.28	0/829	0.51	0/1107
43	q	0.27	0/864	0.51	0/1156
44	r	0.26	0/744	0.45	0/994
45	s	0.32	0/787	0.49	0/1051
46	t	0.28	0/766	0.46	0/1025
47	u	0.29	0/582	0.47	0/769
48	v	0.27	0/635	0.45	0/848
49	w	0.35	0/510	0.44	0/677
5	E	0.30	0/1735	0.46	0/2338
50	x	0.25	0/453	0.45	0/605
51	y	0.25	0/450	0.46	0/599
52	z	0.26	0/416	0.48	0/554
53	0	0.27	0/380	0.46	0/498
54	1	0.26	0/513	0.56	0/676
55	2	0.28	0/303	0.51	0/397
56	3	0.28	0/1001	0.51	0/1350
57	4	0.27	0/531	0.47	0/709
6	F	0.28	0/1651	0.49	0/2225
7	G	0.31	0/1665	0.48	0/2227
8	H	0.28	0/1154	0.51	0/1554
9	I	0.28	0/835	0.51	0/1128
All	All	0.30	10/158671 (0.0%)	0.76	50/237100 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	3	3
23	W	0	1
40	n	0	1
5	E	0	1
56	3	0	2
All	All	3	8

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1	G	OP3-P	-11.91	1.46	1.61
25	Y	1	G	OP3-P	-10.62	1.48	1.61
26	Z	1	U	OP3-P	-10.58	1.48	1.61
2	B	1	C	OP3-P	-10.57	1.48	1.61
29	c	128	ALA	C-N	10.24	1.53	1.34

The worst 5 of 50 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	15	G	N1-C6-O6	-9.46	114.22	119.90
4	D	436	C	N3-C2-O2	-8.68	115.82	121.90
4	D	495	A	O4'-C1'-N9	8.13	114.71	108.20
25	Y	1941	C	C2-N1-C1'	7.93	127.53	118.80
4	D	492	C	N3-C2-O2	-7.78	116.45	121.90

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	15	G	C4',C2',C3'

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	13	U	Sidechain
1	A	17	G	Sidechain
1	A	18	C	Sidechain
5	E	87	ASP	Peptide
23	W	68	LYS	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	621	0	310	110	0
2	B	1623	0	822	73	0
3	C	362	0	368	73	0
4	D	33028	0	16644	613	0
5	E	1704	0	1732	49	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	F	1624	0	1699	28	0
7	G	1643	0	1708	65	0
8	H	1141	0	1170	61	0
9	I	817	0	808	28	0
10	J	1181	0	1240	33	0
11	K	979	0	1034	22	0
12	L	1022	0	1070	39	0
13	M	786	0	828	33	0
14	N	869	0	878	37	0
15	O	955	0	1019	20	0
16	P	883	0	944	25	0
17	Q	799	0	841	28	0
18	R	714	0	737	9	0
19	S	649	0	666	14	0
20	T	648	0	691	16	0
21	U	504	0	502	12	0
22	V	637	0	665	15	0
23	W	665	0	714	30	0
24	X	495	0	486	23	0
25	Y	62338	0	31376	1203	0
26	Z	2572	0	1302	43	0
27	a	2082	0	2157	0	0
28	b	1565	0	1616	0	0
29	c	1552	0	1619	0	0
30	d	1410	0	1447	0	0
31	e	1323	0	1374	0	0
32	f	1111	0	1148	0	0
33	g	1032	0	1088	0	0
34	h	1129	0	1162	0	0
35	i	938	0	1012	0	0
36	j	1045	0	1117	0	0
37	k	1074	0	1157	0	0
38	l	960	0	1000	0	0
39	m	892	0	923	0	0
40	n	917	0	965	0	0
41	o	947	0	1022	0	0
42	p	816	0	839	0	0
43	q	857	0	922	0	0
44	r	738	0	807	0	0
45	s	779	0	834	0	0
46	t	753	0	780	0	0
47	u	575	0	592	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
48	v	625	0	655	0	0
49	w	509	0	543	0	0
50	x	449	0	491	0	0
51	y	444	0	461	0	0
52	z	409	0	440	0	0
53	0	377	0	418	14	0
54	1	504	0	574	13	0
55	2	302	0	343	7	0
56	3	988	0	1025	78	0
57	4	522	0	522	20	0
All	All	146883	0	99307	2613	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

The worst 5 of 2613 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:17:C:H4'	2:B:18:G:C5'	1.44	1.44
1:A:26:A:H62	8:H:19:ARG:NH1	1.15	1.41
1:A:26:A:H62	8:H:19:ARG:CZ	1.32	1.40
2:B:17:C:N3	2:B:61:C:H5'	1.22	1.40
1:A:27:G:H2'	1:A:28:A:C8	1.59	1.38

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	44/46 (96%)	37 (84%)	6 (14%)	1 (2%)	7	46
5	E	216/218 (99%)	177 (82%)	39 (18%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	F	204/206 (99%)	178 (87%)	26 (13%)	0	100	100
7	G	203/205 (99%)	162 (80%)	41 (20%)	0	100	100
8	H	155/157 (99%)	128 (83%)	24 (16%)	3 (2%)	9	50
9	I	98/100 (98%)	79 (81%)	18 (18%)	1 (1%)	18	62
10	J	149/151 (99%)	124 (83%)	25 (17%)	0	100	100
11	K	127/129 (98%)	107 (84%)	19 (15%)	1 (1%)	22	65
12	L	125/127 (98%)	95 (76%)	29 (23%)	1 (1%)	22	65
13	M	96/98 (98%)	75 (78%)	20 (21%)	1 (1%)	18	62
14	N	114/116 (98%)	97 (85%)	16 (14%)	1 (1%)	20	64
15	O	121/123 (98%)	101 (84%)	20 (16%)	0	100	100
16	P	112/114 (98%)	91 (81%)	21 (19%)	0	100	100
17	Q	99/101 (98%)	75 (76%)	24 (24%)	0	100	100
18	R	86/88 (98%)	66 (77%)	20 (23%)	0	100	100
19	S	80/82 (98%)	66 (82%)	14 (18%)	0	100	100
20	T	78/80 (98%)	69 (88%)	9 (12%)	0	100	100
21	U	63/65 (97%)	52 (82%)	10 (16%)	1 (2%)	11	53
22	V	77/79 (98%)	66 (86%)	11 (14%)	0	100	100
23	W	83/85 (98%)	66 (80%)	17 (20%)	0	100	100
24	X	63/65 (97%)	41 (65%)	21 (33%)	1 (2%)	11	53
27	a	269/271 (99%)	241 (90%)	28 (10%)	0	100	100
28	b	207/209 (99%)	184 (89%)	23 (11%)	0	100	100
29	c	199/201 (99%)	172 (86%)	26 (13%)	1 (0%)	32	73
30	d	175/177 (99%)	151 (86%)	24 (14%)	0	100	100
31	e	174/176 (99%)	153 (88%)	21 (12%)	0	100	100
32	f	147/149 (99%)	121 (82%)	24 (16%)	2 (1%)	13	56
33	g	139/141 (99%)	114 (82%)	22 (16%)	3 (2%)	8	47
34	h	140/142 (99%)	129 (92%)	7 (5%)	4 (3%)	5	41
35	i	120/122 (98%)	108 (90%)	11 (9%)	1 (1%)	22	65
36	j	141/143 (99%)	121 (86%)	18 (13%)	2 (1%)	13	56
37	k	134/136 (98%)	116 (87%)	18 (13%)	0	100	100
38	l	118/120 (98%)	98 (83%)	19 (16%)	1 (1%)	22	65

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
39	m	114/116 (98%)	92 (81%)	21 (18%)	1 (1%)	20	64
40	n	112/114 (98%)	103 (92%)	9 (8%)	0	100	100
41	o	115/117 (98%)	92 (80%)	23 (20%)	0	100	100
42	p	101/103 (98%)	89 (88%)	11 (11%)	1 (1%)	18	62
43	q	108/110 (98%)	92 (85%)	16 (15%)	0	100	100
44	r	91/93 (98%)	74 (81%)	17 (19%)	0	100	100
45	s	100/102 (98%)	89 (89%)	11 (11%)	0	100	100
46	t	92/94 (98%)	85 (92%)	7 (8%)	0	100	100
47	u	73/75 (97%)	69 (94%)	4 (6%)	0	100	100
48	v	75/77 (97%)	67 (89%)	8 (11%)	0	100	100
49	w	61/63 (97%)	49 (80%)	12 (20%)	0	100	100
50	x	56/58 (97%)	49 (88%)	6 (11%)	1 (2%)	10	51
51	y	54/56 (96%)	49 (91%)	4 (7%)	1 (2%)	9	50
52	z	48/50 (96%)	42 (88%)	5 (10%)	1 (2%)	8	48
53	0	44/46 (96%)	35 (80%)	9 (20%)	0	100	100
54	1	62/64 (97%)	56 (90%)	6 (10%)	0	100	100
55	2	36/38 (95%)	32 (89%)	4 (11%)	0	100	100
56	3	129/131 (98%)	102 (79%)	23 (18%)	4 (3%)	5	40
57	4	64/66 (97%)	53 (83%)	11 (17%)	0	100	100
All	All	5891/5995 (98%)	4979 (84%)	878 (15%)	34 (1%)	33	70

5 of 34 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	45	ASP
34	h	81	ILE
52	z	4	ILE
8	H	122	VAL
39	m	35	ILE

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	42/42 (100%)	42 (100%)	0	100	100
5	E	180/180 (100%)	180 (100%)	0	100	100
6	F	170/170 (100%)	170 (100%)	0	100	100
7	G	172/172 (100%)	172 (100%)	0	100	100
8	H	114/119 (96%)	114 (100%)	0	100	100
9	I	87/87 (100%)	87 (100%)	0	100	100
10	J	124/124 (100%)	124 (100%)	0	100	100
11	K	104/104 (100%)	104 (100%)	0	100	100
12	L	105/105 (100%)	105 (100%)	0	100	100
13	M	86/86 (100%)	86 (100%)	0	100	100
14	N	89/89 (100%)	89 (100%)	0	100	100
15	O	103/103 (100%)	103 (100%)	0	100	100
16	P	92/92 (100%)	92 (100%)	0	100	100
17	Q	79/83 (95%)	79 (100%)	0	100	100
18	R	76/76 (100%)	76 (100%)	0	100	100
19	S	65/65 (100%)	65 (100%)	0	100	100
20	T	74/74 (100%)	74 (100%)	0	100	100
21	U	48/56 (86%)	48 (100%)	0	100	100
22	V	70/70 (100%)	70 (100%)	0	100	100
23	W	65/65 (100%)	65 (100%)	0	100	100
24	X	44/55 (80%)	44 (100%)	0	100	100
27	a	216/216 (100%)	214 (99%)	2 (1%)	82	92
28	b	164/164 (100%)	164 (100%)	0	100	100
29	c	165/165 (100%)	165 (100%)	0	100	100
30	d	148/148 (100%)	148 (100%)	0	100	100
31	e	137/137 (100%)	137 (100%)	0	100	100
32	f	114/114 (100%)	114 (100%)	0	100	100
33	g	109/109 (100%)	109 (100%)	0	100	100
34	h	116/116 (100%)	116 (100%)	0	100	100
35	i	103/103 (100%)	103 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	j	102/102 (100%)	102 (100%)	0	100	100
37	k	109/109 (100%)	109 (100%)	0	100	100
38	l	100/100 (100%)	100 (100%)	0	100	100
39	m	86/86 (100%)	86 (100%)	0	100	100
40	n	99/99 (100%)	99 (100%)	0	100	100
41	o	89/89 (100%)	89 (100%)	0	100	100
42	p	84/84 (100%)	84 (100%)	0	100	100
43	q	93/93 (100%)	93 (100%)	0	100	100
44	r	80/80 (100%)	80 (100%)	0	100	100
45	s	83/83 (100%)	83 (100%)	0	100	100
46	t	78/78 (100%)	78 (100%)	0	100	100
47	u	57/57 (100%)	57 (100%)	0	100	100
48	v	67/67 (100%)	67 (100%)	0	100	100
49	w	55/55 (100%)	55 (100%)	0	100	100
50	x	48/48 (100%)	48 (100%)	0	100	100
51	y	47/47 (100%)	47 (100%)	0	100	100
52	z	45/45 (100%)	45 (100%)	0	100	100
53	0	38/38 (100%)	38 (100%)	0	100	100
54	1	51/51 (100%)	51 (100%)	0	100	100
55	2	34/34 (100%)	34 (100%)	0	100	100
56	3	100/100 (100%)	100 (100%)	0	100	100
57	4	59/59 (100%)	59 (100%)	0	100	100
All	All	4865/4893 (99%)	4863 (100%)	2 (0%)	100	100

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
27	a	85	ASN
27	a	259	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	28/29 (96%)	14 (50%)	8 (28%)
2	B	75/76 (98%)	18 (24%)	3 (4%)
25	Y	2898/2903 (99%)	673 (23%)	123 (4%)
26	Z	119/120 (99%)	22 (18%)	6 (5%)
4	D	1535/1539 (99%)	327 (21%)	58 (3%)
All	All	4655/4667 (99%)	1054 (22%)	198 (4%)

5 of 1054 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	6	A
1	A	7	U
1	A	8	A
1	A	15	G
1	A	16	G

5 of 198 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
25	Y	464	U
25	Y	971	G
25	Y	2790	U
25	Y	507	A
25	Y	704	G

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

35 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
4	2MG	D	1207	4	19,26,27	4.73	7 (36%)	20,38,41	2.13	7 (35%)
4	4OC	D	1402	4	16,23,24	0.80	0	19,32,35	1.16	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	5MC	D	1407	4	15,22,23	3.11	5 (33%)	17,32,35	1.25	2 (11%)
4	UR3	D	1498	4	14,22,23	2.83	4 (28%)	16,32,35	0.65	0
4	2MG	D	1516	4	19,26,27	4.74	7 (36%)	20,38,41	2.17	8 (40%)
4	MA6	D	1518	4	16,26,27	1.07	1 (6%)	18,38,41	3.49	4 (22%)
4	MA6	D	1519	4	16,26,27	1.04	1 (6%)	18,38,41	3.52	4 (22%)
4	PSU	D	516	4	16,21,22	1.17	3 (18%)	20,30,33	3.47	6 (30%)
4	7MG	D	527	4	20,26,27	4.39	8 (40%)	22,39,42	1.72	8 (36%)
4	2MG	D	966	4	19,26,27	4.72	7 (36%)	20,38,41	2.35	8 (40%)
4	5MC	D	967	4	15,22,23	3.26	5 (33%)	17,32,35	1.16	2 (11%)
25	6MZ	Y	1618	25	18,25,26	2.14	3 (16%)	16,36,39	2.74	3 (18%)
25	2MG	Y	1835	25	19,26,27	4.69	7 (36%)	20,38,41	2.16	7 (35%)
25	PSU	Y	1911	25	16,21,22	1.13	2 (12%)	20,30,33	3.43	6 (30%)
25	3TD	Y	1915	25	16,22,23	3.82	5 (31%)	19,32,35	1.87	3 (15%)
25	PSU	Y	1917	25	16,21,22	1.13	2 (12%)	20,30,33	3.42	6 (30%)
25	5MU	Y	1939	25	14,22,23	1.57	2 (14%)	16,32,35	2.71	3 (18%)
25	5MC	Y	1962	25	15,22,23	3.30	5 (33%)	17,32,35	1.01	2 (11%)
25	6MZ	Y	2030	25	18,25,26	2.10	3 (16%)	16,36,39	3.01	3 (18%)
25	7MG	Y	2069	25	20,26,27	4.36	8 (40%)	22,39,42	1.65	7 (31%)
25	OMG	Y	2251	25,2	18,26,27	3.52	7 (38%)	22,38,41	2.03	5 (22%)
25	2MG	Y	2445	25	19,26,27	4.72	7 (36%)	20,38,41	2.23	8 (40%)
25	H2U	Y	2449	25	17,21,22	3.13	5 (29%)	21,30,33	2.84	5 (23%)
25	PSU	Y	2457	25	16,21,22	1.14	2 (12%)	20,30,33	3.49	6 (30%)
25	OMC	Y	2498	25	15,22,23	3.49	6 (40%)	19,31,34	0.73	0
25	2MA	Y	2503	25	18,25,26	3.52	5 (27%)	17,37,40	1.47	3 (17%)
25	PSU	Y	2504	25	16,21,22	1.51	3 (18%)	20,30,33	3.64	6 (30%)
25	OMU	Y	2552	25	14,22,23	3.42	5 (35%)	18,31,34	1.74	1 (5%)
25	PSU	Y	2580	25	16,21,22	1.09	1 (6%)	20,30,33	3.65	8 (40%)
25	PSU	Y	2604	25	16,21,22	1.14	2 (12%)	20,30,33	3.46	6 (30%)
25	PSU	Y	2605	25	16,21,22	1.11	2 (12%)	20,30,33	3.47	6 (30%)
25	1MG	Y	745	25	18,26,27	3.60	5 (27%)	18,39,42	2.27	2 (11%)
25	PSU	Y	746	25	16,21,22	1.09	2 (12%)	20,30,33	3.51	7 (35%)
25	5MC	Y	747	25	15,22,23	3.25	5 (33%)	17,32,35	1.03	1 (5%)
25	PSU	Y	955	25	16,21,22	1.13	2 (12%)	20,30,33	3.46	6 (30%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	2MG	D	1207	4	-	0/5/27/28	0/3/3/3
4	4OC	D	1402	4	-	0/7/29/30	0/2/2/2
4	5MC	D	1407	4	-	0/3/25/26	0/2/2/2
4	UR3	D	1498	4	-	0/3/25/26	0/2/2/2
4	2MG	D	1516	4	-	0/5/27/28	0/3/3/3
4	MA6	D	1518	4	-	0/7/29/30	0/3/3/3
4	MA6	D	1519	4	-	0/7/29/30	0/3/3/3
4	PSU	D	516	4	-	0/7/25/26	0/2/2/2
4	7MG	D	527	4	-	0/7/37/38	0/3/3/3
4	2MG	D	966	4	-	0/5/27/28	0/3/3/3
4	5MC	D	967	4	-	0/3/25/26	0/2/2/2
25	6MZ	Y	1618	25	-	0/5/27/28	0/3/3/3
25	2MG	Y	1835	25	-	0/5/27/28	0/3/3/3
25	PSU	Y	1911	25	-	0/7/25/26	0/2/2/2
25	3TD	Y	1915	25	-	0/7/25/26	0/2/2/2
25	PSU	Y	1917	25	-	0/7/25/26	0/2/2/2
25	5MU	Y	1939	25	-	0/3/25/26	0/2/2/2
25	5MC	Y	1962	25	-	0/3/25/26	0/2/2/2
25	6MZ	Y	2030	25	-	0/5/27/28	0/3/3/3
25	7MG	Y	2069	25	-	0/7/37/38	0/3/3/3
25	OMG	Y	2251	25,2	-	0/5/27/28	0/3/3/3
25	2MG	Y	2445	25	-	0/5/27/28	0/3/3/3
25	H2U	Y	2449	25	-	0/7/38/39	0/2/2/2
25	PSU	Y	2457	25	-	0/7/25/26	0/2/2/2
25	OMC	Y	2498	25	-	0/5/27/28	0/2/2/2
25	2MA	Y	2503	25	-	0/3/25/26	0/3/3/3
25	PSU	Y	2504	25	-	0/7/25/26	0/2/2/2
25	OMU	Y	2552	25	-	0/5/27/28	0/2/2/2
25	PSU	Y	2580	25	-	0/7/25/26	0/2/2/2
25	PSU	Y	2604	25	-	0/7/25/26	0/2/2/2
25	PSU	Y	2605	25	-	0/7/25/26	0/2/2/2
25	1MG	Y	745	25	-	0/3/25/26	0/3/3/3
25	PSU	Y	746	25	-	0/7/25/26	0/2/2/2
25	5MC	Y	747	25	-	0/3/25/26	0/2/2/2
25	PSU	Y	955	25	-	0/7/25/26	0/2/2/2

The worst 5 of 144 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	Y	1915	3TD	C5-C1'	-7.22	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	Y	1939	5MU	C4-N3	-4.72	1.24	1.33
25	Y	2504	PSU	C5-C1'	-4.41	1.48	1.52
25	Y	1835	2MG	O6-C6	-2.96	1.17	1.24
25	Y	2030	6MZ	C5-C4	-2.95	1.33	1.40

The worst 5 of 160 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	Y	2580	PSU	N1-C2-N3	-11.50	120.13	128.40
25	Y	2457	PSU	N1-C2-N3	-11.46	120.16	128.40
4	D	516	PSU	N1-C2-N3	-11.37	120.22	128.40
25	Y	746	PSU	N1-C2-N3	-11.34	120.24	128.40
25	Y	1917	PSU	N1-C2-N3	-11.27	120.29	128.40

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

20 monomers are involved in 50 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	1402	4OC	7	0
4	D	1407	5MC	4	0
4	D	1498	UR3	4	0
4	D	1518	MA6	4	0
4	D	1519	MA6	2	0
4	D	527	7MG	1	0
4	D	966	2MG	2	0
4	D	967	5MC	2	0
25	Y	1835	2MG	2	0
25	Y	1911	PSU	1	0
25	Y	1939	5MU	1	0
25	Y	1962	5MC	2	0
25	Y	2251	OMG	4	0
25	Y	2449	H2U	1	0
25	Y	2498	OMC	1	0
25	Y	2503	2MA	2	0
25	Y	2580	PSU	6	0
25	Y	745	1MG	4	0
25	Y	746	PSU	2	0
25	Y	955	PSU	2	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.